Effect of positronium formation on elastic e^+-H scattering at medium energies

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(Received 3 December 1987)

Elastic e^+-H scattering has been investigated by a perturbative approach at medium energies. The effect of the positronium-formation channel on the elastic one has been taken into account explicitly. In the perturbative series, the first term is the solution of the coupled static equation. The conventional perturbative series including the rearrangement channel has also been employed. The effect of the capture channel on the elastic one is found to enhance the cross section near the forward direction. The present results are compared with existing elaborate theoretical predictions.

I. INTRODUCTION

The past decade has witnessed the maturity of positron-collision physics as an important field of science. Intense and energy-resolved positron beams make it possible to perform electron- and positron-collision experiments almost on an equal footing. Very recently, experiments have been planned to measure ionization and positronium-formation cross sections in e^+-H collisions.[1] Total and elastic cross sections in e^+-H scattering are expected to be measured in the near future.

There are three elaborate studies[2-4] to investigate e^+-H scattering that are especially germane. Byron *et al.*[2] have employed a unitarized eikonal Born series to calculate elastic and excitation cross sections of e^+-H scattering at intermediate and high energies. Bransden *et al.*[3] have investigated these processes using the coupled-channel-optical method. In their calculations. Bransden *et al.* have taken six eigenstates explicitly, and the effects of higher excited and continuum states are included in an approximate way. Most recently, Walters[4] has predicted elastic, ($1s$-$2s$) and ($1s$-$2p$) excitation cross sections using the multipseudostate-close-coupling approximation in which 3 eigenstates and 18 pseudostates have been employed. In these three calculations, the effect of the positronium-formation channel on the direct channel has not been taken into account. This effect is expected to contribute at intermediate energies. Moreover, the effects of the higher excited and continuum states are also important (Walters[4]). To have a reliable calculation, it is expected that these two effects should be taken into account in predicting the elastic cross section at intermediate and high energies.

We consider elastic e^+-H scattering at medium and high energies. Our main motivation is to estimate the effect of the positronium-formation channel on the elastic one. We employ two perturbative series retaining up to the second-order term in both the direct and rearrangement channels. In our first model, the unperturbative term is the solution of the coupled state equation. This model is similar to that of Kingston and Walters.[5] Moreover, we have calculated the conventional perturbative series in which the second-order rearrangement terms provide the effect of the positronium-formation channel on the elastic one. We report the total integrated and differential cross sections in the energy range 30–300 eV.

II. THEORY

In the present calculation, we plan to retain up to the second-order term both in the direct and rearrangement channels. In the conventional perturbative approach, the elastic scattering amplitude up to the second-order term is given by Ghosh *et al.*[6] and Basu *et al.*[7]

$$f_{1s,1s}(\mathbf{k}',\mathbf{k})=f^{B}_{1s,1s}(\mathbf{k}',\mathbf{k})+f^{B2}_{1s,1s}(\mathbf{k}',\mathbf{k})+g^{B2}_{1s,1s}(\mathbf{k}',\mathbf{k}) , \tag{1}$$

where

$$f^{B2}_{1s,1s}(\mathbf{k}',\mathbf{k})=\frac{1}{2\pi^2}\sum_{n''}\int d\mathbf{k}''\frac{f^{B}_{1s,n''}(\mathbf{k}',\mathbf{k}'')f^{B}_{n'',1s}(\mathbf{k}'',\mathbf{k})}{k''^2-k^2_{n''}+i\epsilon} , \tag{2}$$

$$g^{B2}_{1s,1s}(\mathbf{k}',\mathbf{k})=\frac{1}{2\pi^2}\sum_{\nu''}\int d\mathbf{k}''\frac{g^{B}_{1s,\nu''}(\mathbf{k}',\mathbf{k}'')g^{B}_{\nu'',1s}(\mathbf{k}'',\mathbf{k})}{k''^2-k^2_{\nu''}+i\epsilon} , \tag{3}$$

with

$$f^{B}_{n',n}(\mathbf{k}',\mathbf{k})=-\frac{\mu_{n'}}{2\pi}\int e^{-i\mathbf{k}'\cdot\mathbf{r}_1}\Phi^*_{n'}(\mathbf{r}_2)\left[\frac{1}{r_1}-\frac{1}{r_{12}}\right]\times\Phi_n(\mathbf{r}_2)e^{i\mathbf{k}\cdot\mathbf{r}_1}d\mathbf{r}_1d\mathbf{r}_2$$

and

$$g^{B}_{\nu',n}(\mathbf{k}',\mathbf{k})=-\frac{\mu_{\nu'}}{2\pi}\int e^{-(i/2)\mathbf{k}'\cdot(\mathbf{r}_1+\mathbf{r}_2)}\eta^*_{\nu'}(\mathbf{r}_{12})\times(H-E)\Phi_n(\mathbf{r}_2)e^{i\mathbf{k}\cdot\mathbf{r}_1}d\mathbf{r}_1d\mathbf{r}_2 .$$

TABLE I. Second-order amplitude g^{B2} with different sets of intermediate states of the positronium atom. Powers of ten are in brackets. R represents the real part of the amplitude. I represents the imaginary part of the amplitude.

Energy (eV)	Angle (deg)	1s R	1s I	1s,2s R	1s,2s I	1s,2s,2p R	1s,2s,2p I
30.0	0.0	−0.2274	0.6119	−0.2259	0.6806	−0.2115	0.7728
	30.0	−0.1116	0.1774	−0.1142	0.2001	−0.1188	0.2168
	120.0	−0.3636[−1]	0.6318[−1]	−0.3673[−1]	0.6916[−1]	−0.3718[−1]	0.7789[−1]
50.0	0.0	−0.2186	0.2224	−0.2397	0.2538	−0.2434	0.2677
	30.0	−0.5542[−1]	0.3272[−1]	−0.6031[−1]	0.3745[−1]	−0.6325[−1]	0.3899[−1]
	120.0	−0.2594[−1]	0.1700[−1]	−0.2804[−1]	0.1936[−1]	−0.2983[−1]	0.2120[−1]
100.0	0.0	−0.7612[−1]	0.3107[−1]	−0.8579[−1]	0.3573[−1]	−0.8748[−1]	0.3699[−1]
	30.0	−0.9889[−2]	0.1185[−2]	−0.1087[−1]	0.1326[−2]	−0.1127[−1]	0.1290[−2]
	120.0	−0.6678[−2]	0.1372[−2]	−0.7393[−2]	0.1583[−2]	−0.7743[−2]	0.1669[−2]

TABLE II. Differential cross section for elastic e^+-H scattering, in units of a_0^2 sr^{-1}. Powers of ten are in brackets.

Angle (deg)	30 eV MBG	30 eV M1	30 eV M2	50 eV MBG	50 eV M1	50 eV M2
0	4.24	6.90	7.82	3.15	3.93	4.09
10	2.34	4.87	5.29	1.60	2.57	2.62
20	1.22	2.83	2.88	8.14[−1]	1.39	1.36
30	6.68[−1]	1.50	1.35	4.52[−1]	7.29[−1]	6.63[−1]
40	3.90[−1]	8.08[−1]	8.44[−1]	2.64[−1]	4.09[−1]	3.33[−1]
50	2.42[−1]	4.84[−1]	3.00[−1]	1.62[−1]	2.58[−1]	1.85[−1]
60	1.58[−1]	3.35[−1]	1.68[−1]	1.04[−1]	1.82[−1]	1.13[−1]
80	7.86[−2]	2.29[−1]	8.13[−2]	4.65[−2]	1.15[−1]	5.23[−2]
100	4.63[−2]	1.95[−1]	5.84[−2]	2.67[−2]	8.88[−2]	2.87[−2]
120	3.09[−2]	1.78[−1]	4.84[−2]	1.68[−2]	6.35[−2]	1.81[−2]
140	2.30[−2]	1.64[−1]	4.38[−2]	1.24[−2]	5.44[−2]	1.37[−2]
160	1.91[−2]	1.56[−1]	4.10[−2]	1.03[−2]	4.93[−2]	1.11[−2]
180	1.80[−2]	1.54[−1]	4.10[−2]	9.73[−3]	4.77[−2]	1.12[−2]

TABLE III. Differential cross section for elastic e^+-H scattering, in units of a_0^2 sr^{-1}. Powers of ten are in brackets.

Angle (deg)	100 eV MBG	100 eV M1	100 eV M2	200 eV MBG	200 eV M1	200 eV M2	300 eV M2
0	2.13	2.27	2.21	1.51	1.56	1.51	1.29
10	1.04	1.30	1.22	7.57[−1]	8.33[−1]	7.81[−1]	6.30[−1]
20	5.21[−1]	6.65[−1]	6.06[−1]	3.18[−1]	3.59[−1]	3.28[−1]	2.16[−1]
30	2.66[−1]	3.41[−1]	2.93[−1]	1.28[−1]	1.51[−1]	1.31[−1]	7.83[−2]
40	1.39[−1]	1.85[−1]	1.47[−1]	5.56[−2]	6.93[−2]	5.66[−2]	2.91[−2]
50	7.59[−2]	1.08[−1]	7.96[−2]	2.70[−2]	3.59[−2]	2.74[−2]	1.34[−2]
60	4.42[−2]	6.90[−2]	4.64[−2]	1.46[−2]	2.08[−2]	1.48[−2]	7.09[−3]
80	1.82[−2]	3.42[−2]	1.88[−2]	5.63[−3]	9.11[−3]	5.65[−3]	2.68[−3]
100	9.50[−3]	2.08[−2]	9.89[−3]	2.86[−3]	5.10[−3]	2.87[−3]	1.35[−3]
120	5.97[−3]	1.47[−2]	6.07[−3]	1.80[−3]	3.39[−3]	1.77[−3]	8.32[−4]
140	4.37[−3]	1.16[−2]	4.52[−3]	1.29[−3]	2.59[−3]	1.29[−3]	6.02[−4]
160	3.66[−3]	1.02[−2]	3.68[−3]	1.08[−3]	2.22[−3]	1.06[−3]	5.00[−4]
180	3.45[−3]	9.75[−3]	3.68[−3]	1.01[−3]	2.11[−3]	1.03[−3]	4.70[−4]

TABLE IV. Total elastic cross section (in units of a_0^2) for e^+-H scattering. Powers of ten are in brackets.

Energy (eV)	Present results M2	Byron *et al.*[a]	Bransden *et al.*[b]
30	4.46		
50	2.22		6.7[−1][c]
100	9.71[−1]	6.90[−1]	5.2[−1]
200	4.78[−1]	4.12[−1]	3.8[−1]
300	3.17[−1]	2.92[−1]	

[a]Reference 2.
[b]Reference 3.
[c]54.42-eV results.

The μ_i's are the reduced mass in the final channel. Here Φ_n and η_ν are the ground-state wave functions of the hydrogen and positronium atoms, and H is the rearrangement Hamiltonian of the system.

Following the method of Kingston and Walters[5] we propose to calculate the scattering amplitude as

$$f_{1s,1s}=f^{\rm CS}_{1s,1s}+\tilde{f}^{\,B2}_{1s,1s}+\tilde{g}^{\,B2}_{1s,1s}\ , \tag{4}$$

where $f^{\rm CS}_{n,n}$ is the solution of the coupled static equation. In $\tilde{f}^{\,B2}$ and $\tilde{g}^{\,B2}$ the summations over n'' and ν'' exclude the ground states of the respective targets. We have evaluated the two scattering amplitudes given by the relations (1) and (4) and denoted them by M1 and M2, respectively. We hasten to add that our model $M2$ is our main model. The second Born term f^{B2} is calculated by retaining two eigenstates ($1s,2s$) and two pseudostates ($2\bar{p},3\bar{s}$). In g^{B2} we have included three eigenstates ($1s,2s,2p$) only.

III. RESULTS AND DISCUSSIONS

The convergence of f^{B2} is examined by Mukherjee *et al.*[8] They have found that their second Born results are in fair agreement with the exact results and with the distorted-wave second Born results of Kingston and Walters[5] in the forward direction. Table I in which are listed the second-order amplitudes g^{B2} with different sets of intermediate states of the positronium atom at three incident energies, provides the measure of convergence of the second Born rearrangement amplitude. We should like to point out another important feature regarding g^{B2}. The major contribution to g^{B2} comes from the $1s$ state of the positronium atom as the intermediate one. This reveals that the effect of g^{B2} is short-ranged in nature. This confirms the findings of Callaway *et al.*[9]

We tabulate the elastic differential cross sections for e^+-H scattering at five incident energies using two models in Tables II and III. The results denoted by MBG are from Mukherjee *et al.*[8] The difference between the present two sets of results and those of Mukherjee *et al.* suggests that the effect of the positronium-formation channel on the elastic one is very significant at all scatter-

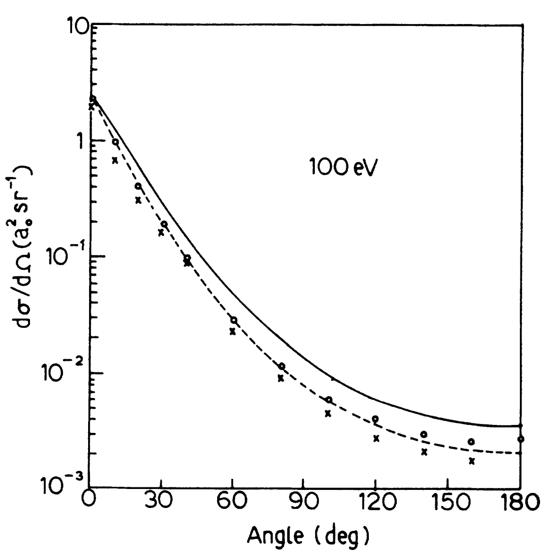

FIG. 1. Differential cross section for positron–hydrogen-atom scattering at 100 eV; ——, present (M2); — — —, Byron *et al.* (Ref. 2); ○, Walters (Ref. 4); ×, Bransden *et al.* (Ref. 3).

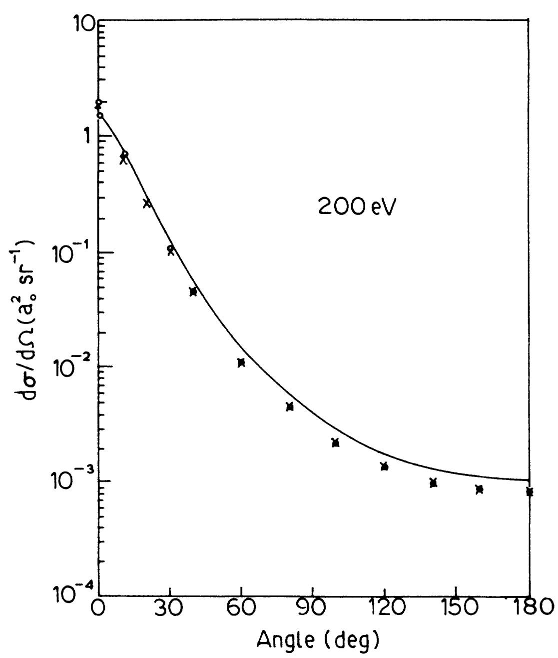

FIG. 2. Differential cross section for positron–hydrogen-atom scattering at 200 eV; ——, present (M2); ○, Byron *et al.* (Ref. 2); ×, Bransden *et al.* (Ref. 3).

TABLE V. Total cross section (in units of a_0^2) for e^+-H scattering.

Energy (eV)	Present results M2	Byron *et al.*[a]	Bransden *et al.*[b]
30	21.09		
50	12.91		7.16[c]
100	6.88	6.84	5.75
200	3.95	4.18	3.65
300	2.88	3.07	

[a]Reference 2.
[b]Reference 3.
[c]54.42-eV results.

ing angles at the lowest energy considered here. The effect decreases with the increase of energy, as expected. At the incident energy 200 eV, the effect is marginal. It may be pointed out that the difference between the two models persists up to 200 eV. The large-angle results suggest that the effect is essentially short-ranged in nature. The sharp increase of the differential cross sections at 30 and 50 eV with the inclusion of the positronium-formation channel is presumably due to the short-range electron-positron correlation (absorption) effect. This is also clear from the fact that imaginary parts of g^{B2} at these energies are appreciable.

Figs. 1 and 2 provide the present differential cross sections (model M2) at 100 and 200 eV along with other theoretical predictions. Except at forward scattering angles, our results are always greater than the other three theoretical predictions. The results of Walters[4] at 100 eV are in good agreement with ours. The present results at 200 eV seem to be in better agreement with those of Byron *et al.*[2] and Bransden *et al.*[3] than at 100 eV.

In Tables IV and V elastic and total cross sections are listed. These tables also include the corresponding results of Byron *et al.*[2] and Bransden *et al.*[3] For incident energy $E \geq 100$ eV the present results are in good agreement with those of Byron *et al.* and Bransden *et al.* Large values at lower energies, we presume, are due to the inclusion of the positronium-formation channel.

We report elastic scattering parameters for positron-hydrogen scattering at medium and high energies, including the effect of the positronium-formation channel explicitly. This effect is found to be appreciable at medium energies. There is room to improve this model. However, the present calculation provides an estimate of this effect. We plan to study positron-hydrogen scattering at medium energies in a more elaborate way in the near future.

ACKNOWLEDGMENT

The authors are thankful to the Authority of the Variable Energy Cyclotron Centre, Calcutta, for allowing us the use of their IRIS-80 computer for the numerical calculations.

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